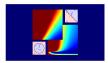
Machine Learning Foundations

(機器學習基石)



Lecture 10: Logistic Regression

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Roadmap

- 1 When Can Machines Learn?
- 2 Why Can Machines Learn?
- **3 How Can Machines Learn?**

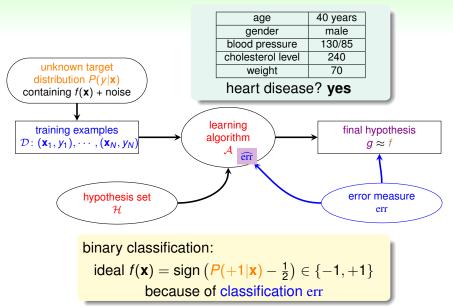
Lecture 9: Linear Regression

analytic solution $\mathbf{w}_{\text{LIN}} = X^{\dagger} \mathbf{y}$ with linear regression hypotheses and squared error

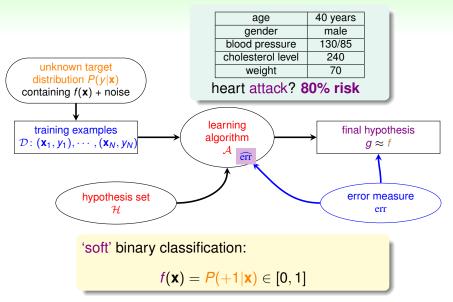
Lecture 10: Logistic Regression

- Logistic Regression Problem
- Logistic Regression Error
- Gradient of Logistic Regression Error
- Gradient Descent
- 4 How Can Machines Learn Better?

Heart Attack Prediction Problem (1/2)



Heart Attack Prediction Problem (2/2)



Soft Binary Classification

target function
$$f(\mathbf{x}) = P(+1|\mathbf{x}) \in [0,1]$$

ideal (noiseless) data

$$\begin{pmatrix} \mathbf{x}_{1}, y'_{1} &= 0.9 &= P(+1|\mathbf{x}_{1}) \\ (\mathbf{x}_{2}, y'_{2} &= 0.2 &= P(+1|\mathbf{x}_{2}) \\ \vdots \\ (\mathbf{x}_{N}, y'_{N} &= 0.6 &= P(+1|\mathbf{x}_{N}) \end{pmatrix}$$

actual (noisy) data

$$\begin{pmatrix} \mathbf{x}_{1}, y_{1} &= \circ & \sim P(y|\mathbf{x}_{1}) \\ (\mathbf{x}_{2}, y_{2} &= \times & \sim P(y|\mathbf{x}_{2}) \end{pmatrix}$$

$$\vdots$$

$$\begin{pmatrix} \mathbf{x}_{N}, y_{N} &= \times & \sim P(y|\mathbf{x}_{N}) \end{pmatrix}$$

same data as hard binary classification, different target function

Soft Binary Classification

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actual (noisy) data

$$\begin{pmatrix} \mathbf{x}_{1}, y'_{1} &= 1 &= \left[\circ \stackrel{?}{\sim} P(y|\mathbf{x}_{1}) \right] \\ \left(\mathbf{x}_{2}, y'_{2} &= 0 &= \left[\circ \stackrel{?}{\sim} P(y|\mathbf{x}_{2}) \right] \right) \\ &\vdots \\ \left(\mathbf{x}_{N}, y'_{N} &= 0 &= \left[\circ \stackrel{?}{\sim} P(y|\mathbf{x}_{N}) \right] \right)$$

same data as hard binary classification, different target function

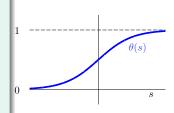
Logistic Hypothesis

age	40 years
gender	male
blood pressure	130/85
cholesterol level	240

• For $\mathbf{x} = (x_0, x_1, x_2, \dots, x_d)$ 'features of patient', calculate a weighted 'risk score':

$$s = \sum_{i=0}^{d} w_i x_i$$

• convert the score to estimated probability by logistic function $\theta(s)$



logistic hypothesis: $h(\mathbf{x}) = \theta(\mathbf{w}^T\mathbf{x})$

Logistic Function



$$\theta(-\infty)=0$$
:

$$\theta(0)=\frac{1}{2};$$

$$\theta(\infty)=1$$

$$\theta(s) = \frac{e^s}{1 + e^s} = \frac{1}{1 + e^{-s}}$$

—smooth, monotonic, sigmoid function of s

logistic regression: use

$$h(\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^T \mathbf{x})}$$

to approximate target function $f(\mathbf{x}) = P(+1|\mathbf{x})$

Fun Time

Logistic Regression and Binary Classification

Consider any logistic hypothesis $h(\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^T \mathbf{x})}$ that approximates $P(y|\mathbf{x})$. 'Convert' $h(\mathbf{x})$ to a binary classification prediction by taking sign $(h(\mathbf{x}) - \frac{1}{2})$. What is the equivalent formula for the binary classification prediction?

- 2 sign $(\mathbf{w}^T \mathbf{x})$
- 3 sign $\left(\mathbf{w}^{\mathsf{T}}\mathbf{x} + \frac{1}{2}\right)$
- 4 none of the above

Reference Answer: (2)

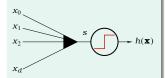
When $\mathbf{w}^{\mathsf{T}}\mathbf{x} = 0$, $h(\mathbf{x})$ is exactly $\frac{1}{2}$. So thresholding $h(\mathbf{x})$ at $\frac{1}{2}$ is the same as thresholding $(\mathbf{w}^{\mathsf{T}}\mathbf{x})$ at 0.

Three Linear Models

linear scoring function: $s = \mathbf{w}^T \mathbf{x}$

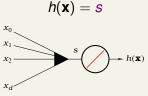
linear classification

$$h(\mathbf{x}) = \operatorname{sign}(\mathbf{s})$$



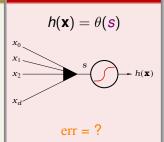
plausible err = 0/1 (small flipping noise)

linear regression



friendly err = squared (easy to minimize)

logistic regression



how to define $E_{in}(\mathbf{w})$ for logistic regression?

Likelihood

target function
$$f(\mathbf{x}) = P(+1|\mathbf{x})$$

$$\Leftrightarrow$$

$$P(y|\mathbf{x}) = \begin{cases} f(\mathbf{x}) & \text{for } y = +1\\ 1 - f(\mathbf{x}) & \text{for } y = -1 \end{cases}$$

consider
$$\mathcal{D} = \{(\mathbf{x}_1, \circ), (\mathbf{x}_2, \times), \dots, (\mathbf{x}_N, \times)\}$$

probability that f generates \mathcal{D}

$$P(\mathbf{x}_1)P(\circ|\mathbf{x}_1) \times P(\mathbf{x}_2)P(\times|\mathbf{x}_2) \times \dots P(\mathbf{x}_N)P(\times|\mathbf{x}_N)$$

likelihood that h generates \mathcal{D}

$$P(\mathbf{x}_1)h(\mathbf{x}_1) \times P(\mathbf{x}_2)(1 - h(\mathbf{x}_2)) \times \dots$$

$$P(\mathbf{x}_N)(1 - h(\mathbf{x}_N))$$

- if *h* ≈ *f*,
 then likelihood(*h*) ≈ probability using *f*
- probability using f usually large

Likelihood

target function
$$f(\mathbf{x}) = P(+1|\mathbf{x})$$

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probability that f generates \mathcal{D}

$$P(\mathbf{x}_1)f(\mathbf{x}_1) \times P(\mathbf{x}_2)(1-f(\mathbf{x}_2)) \times \dots$$

 $P(\mathbf{x}_N)(1-f(\mathbf{x}_N))$

likelihood that h generates \mathcal{D}

$$P(\mathbf{x}_1)h(\mathbf{x}_1) \times P(\mathbf{x}_2)(1-h(\mathbf{x}_2)) \times \dots P(\mathbf{x}_N)(1-h(\mathbf{x}_N))$$

- if *h* ≈ *f*,
 then likelihood(*h*) ≈ probability using *f*
- probability using f usually large

Likelihood of Logistic Hypothesis

likelihood(h) \approx (probability using f) \approx large

$$g = \underset{h}{\operatorname{argmax}} \operatorname{likelihood}(h)$$

when logistic: $h(\mathbf{x}) = \theta(\mathbf{w}^T \mathbf{x})$

$$1 - h(\mathbf{x}) = h(-\mathbf{x})$$



likelihood(h) = $P(\mathbf{x}_1)h(\mathbf{x}_1) \times P(\mathbf{x}_2)(1 - h(\mathbf{x}_2)) \times \dots P(\mathbf{x}_N)(1 - h(\mathbf{x}_N))$

likelihood(logistic
$$h$$
) $\propto \prod_{n=1}^{N} h(y_n \mathbf{x}_n)$

Likelihood of Logistic Hypothesis

likelihood(h) \approx (probability using f) \approx large

$$g = \underset{h}{\operatorname{argmax}} \operatorname{likelihood}(h)$$

when logistic: $h(\mathbf{x}) = \theta(\mathbf{w}^T\mathbf{x})$

$$1 - h(\mathbf{x}) = h(-\mathbf{x})$$



likelihood(
$$h$$
) = $P(\mathbf{x}_1)h(+\mathbf{x}_1) \times P(\mathbf{x}_2)h(-\mathbf{x}_2) \times \dots P(\mathbf{x}_N)h(-\mathbf{x}_N)$

likelihood(logistic
$$h$$
) $\propto \prod_{n=1}^{N} h(y_n \mathbf{x}_n)$

$$\max_{h} \quad \text{likelihood(logistic } h) \propto \prod_{n=1}^{N} h(y_n \mathbf{x}_n)$$

$$\max_{\mathbf{w}} \quad likelihood(\mathbf{w}) \propto \prod_{n=1}^{N} \theta \left(y_n \mathbf{w}^T \mathbf{x}_n \right)$$

$$\max_{\mathbf{w}} \quad \ln \prod_{n=1}^{N} \theta \left(y_{n} \mathbf{w}^{T} \mathbf{x}_{n} \right)$$

$$\frac{1}{N} \sum_{n=1}^{N} - \ln \theta \left(y_n \mathbf{w}^T \mathbf{x}_n \right)$$

$$\theta(s) = \frac{1}{1 + \exp(-s)} : \min_{\mathbf{w}} \frac{1}{N} \sum_{n=1}^{N} \ln\left(1 + \exp(-y_n \mathbf{w}^T \mathbf{x}_n)\right)$$

$$\implies \min_{\mathbf{w}} \frac{1}{N} \sum_{n=1}^{N} \frac{1}{\exp(\mathbf{w}, \mathbf{x}_n, \mathbf{y}_n)}$$

$$E_{\text{in}}(\mathbf{w})$$

$$err(\mathbf{w}, \mathbf{x}, y) = ln(1 + exp(-y\mathbf{w}\mathbf{x})):$$
 cross-entropy error

Fun Time

The four statements below help us understand more about the cross-entropy error $\operatorname{err}(\mathbf{w}, \mathbf{x}, y) = \ln\left(1 + \exp(-y\mathbf{w}^T\mathbf{x})\right)$. Consider $\mathbf{w}^T\mathbf{x} \neq 0$. Which statement is not true?

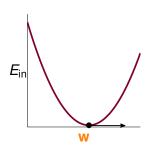
- 1 For any \mathbf{w}, \mathbf{x} , and y, $err(\mathbf{w}, \mathbf{x}, y) > 0$.
- **2** For any **w**, **x**, and *y*, $err(\mathbf{w}, \mathbf{x}, y) < 1126$.
- 3 When $y = \text{sign}(\mathbf{w}^T \mathbf{x}), \text{err}(\mathbf{w}, \mathbf{x}, y) < \ln 2$.
- 4 When $y \neq \text{sign}(\mathbf{w}^T\mathbf{x})$, $\text{err}(\mathbf{w}, \mathbf{x}, y) \geq \ln 2$.

Reference Answer: 2

1126, really? :-) You are highly encouraged to plot the curve of err with respect to some fixed y and some varying score $s = \mathbf{w}^T \mathbf{x}$ to know more about the error measure. After plotting, it is easy to see that err is not bounded above, and the other three choices are correct.

Minimizing $E_{in}(\mathbf{w})$

$$\min_{\mathbf{w}} \quad E_{in}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \ln \left(1 + \exp(-y_n \mathbf{w}^T \mathbf{x}_n) \right)$$



- E_{in}(w): continuous, differentiable, twice-differentiable, convex
- how to minimize? locate valley

want
$$\nabla E_{in}(\mathbf{w}) = \mathbf{0}$$

first: derive $\nabla E_{in}(\mathbf{w})$

The Gradient $\nabla E_{in}(\mathbf{w})$

$$E_{\text{in}}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \ln \left(\underbrace{1 + \exp(-y_n \mathbf{w}^T \mathbf{x}_n)}_{\square} \right)$$

$$\frac{\partial E_{in}(\mathbf{w})}{\partial w_{i}} = \frac{1}{N} \sum_{n=1}^{N} \left(\frac{\partial \ln(\square)}{\partial \square} \right) \left(\frac{\partial (1 + \exp(\bigcirc))}{\partial \bigcirc} \right) \left(\frac{\partial - y_{n} \mathbf{w}^{T} \mathbf{x}_{n}}{\partial w_{i}} \right) \\
= \frac{1}{N} \sum_{n=1}^{N} \left(\frac{\exp(\bigcirc)}{1 + \exp(\bigcirc)} \right) \left(-y_{n} \mathbf{x}_{n,i} \right) = \frac{1}{N} \sum_{n=1}^{N} \theta(\bigcirc) \left(-y_{n} \mathbf{x}_{n,i} \right)$$

$$\nabla E_{\text{in}}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \theta \left(-y_n \mathbf{w}^T \mathbf{x}_n \right) \left(-y_n \mathbf{x}_n \right)$$

The Gradient $\nabla E_{in}(\mathbf{w})$

$$E_{in}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \ln \left(\underbrace{1 + \exp(-y_n \mathbf{w}^T \mathbf{x}_n)}_{\square} \right)$$

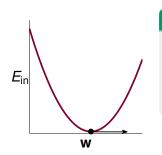
$$\frac{\partial E_{in}(\mathbf{w})}{\partial w_{i}} = \frac{1}{N} \sum_{n=1}^{N} \left(\frac{\partial \ln(\square)}{\partial \square} \right) \left(\frac{\partial (1 + \exp(\bigcirc))}{\partial \bigcirc} \right) \left(\frac{\partial -y_{n} \mathbf{w}^{T} \mathbf{x}_{n}}{\partial w_{i}} \right) \\
= \frac{1}{N} \sum_{n=1}^{N} \left(\frac{1}{\square} \right) \left(\exp(\bigcirc) \right) \left(-y_{n} x_{n,i} \right) \\
= \frac{1}{N} \sum_{n=1}^{N} \left(\frac{\exp(\bigcirc)}{1 + \exp(\bigcirc)} \right) \left(-y_{n} x_{n,i} \right) = \frac{1}{N} \sum_{n=1}^{N} \theta(\bigcirc) \left(-y_{n} x_{n,i} \right)$$

$$\nabla E_{\text{in}}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \theta \left(-y_n \mathbf{w}^T \mathbf{x}_n \right) \left(-y_n \mathbf{x}_n \right)$$

Minimizing $E_{in}(\mathbf{w})$

$$\min_{\mathbf{w}} E_{in}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \ln \left(1 + \exp(-y_n \mathbf{w}^T \mathbf{x}_n) \right)$$

$$\text{want } \nabla E_{in}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \theta \left(-y_n \mathbf{w}^T \mathbf{x}_n \right) \left(-y_n \mathbf{x}_n \right) = \mathbf{0}$$



scaled θ -weighted sum of $-y_n \mathbf{x}_n$

- all $\theta(\cdot) = 0$: only if $y_n \mathbf{w}^T \mathbf{x}_n \gg 0$ —linear separable \mathcal{D}
- weighted sum = 0: non-linear equation of w

closed-form solution? no :-(

PLA Revisited: Iterative Optimization

PLA: start from some \mathbf{w}_0 (say, $\mathbf{0}$), and 'correct' its mistakes on \mathcal{D}

For t = 0, 1, ...

1 find a mistake of \mathbf{w}_t called $(\mathbf{x}_{n(t)}, y_{n(t)})$

$$sign\left(\mathbf{w}_{t}^{\mathsf{T}}\mathbf{x}_{n(t)}\right) \neq y_{n(t)}$$

2 (try to) correct the mistake by

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t + y_{n(t)} \mathbf{x}_{n(t)}$$

when stop, return last \mathbf{w} as g

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$$sign\left(\mathbf{w}_{t}^{T}\mathbf{x}_{n(t)}\right) \neq y_{n(t)}$$

2 (try to) correct the mistake by

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t + y_{n(t)} \mathbf{x}_{n(t)}$$

 \bullet (equivalently) pick some n, and update \mathbf{w}_t by

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t + \left[\operatorname{sign} \left(\mathbf{w}_t^\mathsf{T} \mathbf{x}_n \right) \neq y_n \right] y_n \mathbf{x}_n$$

when stop, return last w as q

PLA Revisited: Iterative Optimization

PLA: start from some \mathbf{w}_0 (say, $\mathbf{0}$), and 'correct' its mistakes on \mathcal{D}

For t = 0, 1, ...

(equivalently) pick some n, and update \mathbf{w}_t by

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t + \underbrace{\mathbf{1}}_{\eta} \cdot \underbrace{\left(\left[\operatorname{sign}\left(\mathbf{w}_t^\mathsf{T} \mathbf{x}_n \right) \neq y_n \right] \cdot y_n \mathbf{x}_n \right)}_{\mathbf{v}}$$

when stop, return last w as g

choice of (η, \mathbf{v}) and stopping condition defines iterative optimization approach

Fun Time

Consider the gradient $\nabla E_{\text{in}}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \theta \left(-y_n \mathbf{w}^T \mathbf{x}_n \right) \left(-y_n \mathbf{x}_n \right)$. That is, each example (\mathbf{x}_n, y_n) contributes to the gradient by an amount of $\theta \left(-y_n \mathbf{w}^T \mathbf{x}_n \right)$. For any given \mathbf{w} , which example contributes the most amount to the gradient?

- 1 the example with the smallest $y_n \mathbf{w}^T \mathbf{x}_n$ value
- 2 the example with the largest $y_n \mathbf{w}^T \mathbf{x}_n$ value
- 3 the example with the smallest $\mathbf{w}^T \mathbf{x}_n$ value
- 4 the example with the largest $\mathbf{w}^T \mathbf{x}_n$ value

Reference Answer: 1

Using the fact that θ is a monotonic function, we see that the example with the smallest $y_n \mathbf{w}^T \mathbf{x}_n$ value contributes to the gradient the most.

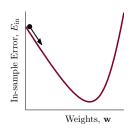
Iterative Optimization

For t = 0, 1, ...

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t + \eta \mathbf{v}$$

when stop, return last w as g

- PLA: v comes from mistake correction
- smooth E_{in}(w) for logistic regression: choose v to get the ball roll 'downhill'?
 - direction v: (assumed) of unit length
 - step size η:
 (assumed) positive



a greedy approach for some given $\eta > 0$:

$$\min_{\|\mathbf{v}\|=1} E_{\text{in}}(\underbrace{\mathbf{w}_t + \frac{\eta \mathbf{v}}{\mathbf{w}_{t+1}}})$$

Linear Approximation

a greedy approach for some given $\eta > 0$:

$$\min_{\|\mathbf{v}\|=1} \quad E_{in}(\mathbf{w}_t + \frac{\eta \mathbf{v}}{\mathbf{v}})$$

- still non-linear optimization, now with constraints
 —not any easier than min_w E_{in}(w)
- · local approximation by linear formula makes problem easier

$$E_{\text{in}}(\mathbf{w}_t + \mathbf{\eta v}) \approx E_{\text{in}}(\mathbf{w}_t) + \mathbf{\eta v}^T \nabla E_{\text{in}}(\mathbf{w}_t)$$

if η really small (Taylor expansion)

an approximate greedy approach for some given small η :

$$\min_{\|\mathbf{v}\|=1} \quad \underbrace{E_{\text{in}}(\mathbf{w}_t)}_{\text{known}} + \underbrace{\eta}_{\text{given positive}} \mathbf{v}^T \underbrace{\nabla E_{\text{in}}(\mathbf{w}_t)}_{\text{known}}$$

Gradient Descent

an approximate greedy approach for some given small η :

$$\min_{\|\mathbf{v}\|=1} \quad \underbrace{E_{\text{in}}(\mathbf{w}_t)}_{\text{known}} + \underbrace{\eta}_{\text{given positive}} \mathbf{v}^T \underbrace{\nabla E_{\text{in}}(\mathbf{w}_t)}_{\text{known}}$$

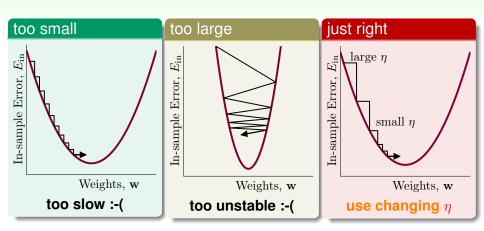
optimal v: opposite direction of ∇E_{in}(v_t)

$$\mathbf{v} = -rac{
abla E_{\mathsf{in}}(\mathbf{w}_t)}{\|
abla E_{\mathsf{in}}(\mathbf{w}_t)\|}$$

• gradient descent: for small η , $\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \eta \frac{\nabla E_{\text{in}}(\mathbf{w}_t)}{\|\nabla E_{\text{in}}(\mathbf{w}_t)\|}$

gradient descent: a simple & popular optimization tool

Choice of η



 η better be monotonic of $\|\nabla E_{in}(\mathbf{w}_t)\|$

Simple Heuristic for Changing η better be monotonic of $\|\nabla E_{in}(\mathbf{w}_t)\|$

• if red $\eta \propto \|\nabla E_{\text{in}}(\mathbf{w}_t)\|$ by ratio purple η

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \frac{\nabla E_{\text{in}}(\mathbf{w}_t)}{\|\nabla E_{\text{in}}(\mathbf{w}_t)\|}$$
 \parallel
 $\mathbf{w}_t - \eta \nabla E_{\text{in}}(\mathbf{w}_t)$

• call purple η the fixed learning rate

fixed learning rate gradient descent:

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \eta \nabla E_{\text{in}}(\mathbf{w}_t)$$

Putting Everything Together

Logistic Regression Algorithm

initialize wo

For
$$t = 0, 1, \dots$$

1 compute

$$\nabla E_{\text{in}}(\mathbf{w}_t) = \frac{1}{N} \sum_{n=1}^{N} \theta \left(-y_n \mathbf{w}_t^T \mathbf{x}_n \right) \left(-y_n \mathbf{x}_n \right)$$

update by

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \eta \nabla E_{\text{in}}(\mathbf{w}_t)$$

...until $\nabla E_{in}(\mathbf{w}_{t+1}) = 0$ or enough iterations return last \mathbf{w}_{t+1} as g

similar time complexity to **pocket** per iteration

Fun Time

If $\mathbf{w}_0 = \mathbf{0}$, and take $\eta = 0.1$. What is \mathbf{w}_1 in the logistic regression algorithm?

$$\mathbf{1} + 0.1 \cdot \frac{1}{N} \sum_{n=1}^{N} y_n \mathbf{x}_n$$

$$2 -0.1 \cdot \frac{1}{N} \sum_{n=1}^{N} y_n \mathbf{x}_n$$

$$\mathbf{3} + 0.05 \cdot \frac{1}{N} \sum_{n=1}^{N} y_n \mathbf{x}_n$$

4
$$-0.05 \cdot \frac{1}{N} \sum_{n=1}^{N} y_n \mathbf{x}_n$$

Reference Answer: (3)

You can do a simple substitution using the fact that $\theta(0) = \frac{1}{2}$. This result shows that a scaled average of $y_n \mathbf{x}_n$ is somewhat 'one-step' better than the zero vector.

Summary

- 1 When Can Machines Learn?
- 2 Why Can Machines Learn?
- **3 How Can Machines Learn?**

Lecture 9: Linear Regression

Lecture 10: Logistic Regression

- Logistic Regression Problem
 P(+1|x) as target and θ(w^Tx) as hypotheses
- Logistic Regression Error cross-entropy (negative log likelihood)
- Gradient of Logistic Regression Error
 θ-weighted sum of data vectors
- Gradient Descent

roll downhill by $-\nabla E_{in}(\mathbf{w})$

- next: linear model'S' for classification
- 4 How Can Machines Learn Better?